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Novel Methods in Terminal Ballistics and Mechanochemistry of Damage

2. Phenomenological Mechanochemistry of Damage in Solid Brittle Dielectrics

by MA Grinfeld

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2. Phenomenological Mechanochemistry of Damage in Solid Brittle Dielectrics

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Weapons and Materials Research Directorate, ARL

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14. ABSTRACT In several promising applications electrostatic forces can reach the intensity that are able to cause plasticity and other types of damage. In this report, we demonstrate how to modify the master system of Phenomenological Mechanochemistry of Damage (PMD) taking such effects into account.					
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1. Introduction

Reasonable understanding of the origin and of the mathematical, physical, and practical roots of the Phenomenological Mechanochemistry of Damage (PMD) is impossible without reading the report on the early history of the PMD.¹ Early publications are deliberately simplified to make transparent the main object and drama of the PMD: it is the competition between the (macroscale) elastic accumulated energy, from one hand, and the (nanoscale) energy, accumulated in the chemical bonds, on the other hand. Because the “multiscale approach” is the buzz word these days, I would like to emphasize that the PMD theory is essentially macroscopic and phenomenological approach, when treating both scales. The PMD is the symbiosis of the damage theory as presented by Kachanov², and of Gibbs’³ variational scheme in thermodynamics of heterogeneous systems as interpreted in the monograph.⁴

Briefly speaking, the PMD theory was born out of the practical necessity to suggest macroscopic models describing the widespread paradoxical radial pattern of damage often observed in terminal ballistics. The radial cracking paradox in ballistics could be formally and technically treated as the manifestation of the typical Stress Driven Rearrangement Instabilities (SDRI) of phase interfaces. The SDRI mechanisms originated as the natural—both physically and mathematically—development of the logically rigorous variational scheme of Gibbs.³ It still remains not understood by the many followers of Gibbs,³ that, when using the Gibbs’³ methodology even in the most rigorous and consistent way, we arrive in 99 out of 100 not to novel physical phenomena but to novel physico/mathematical paradoxes.

Discovery of paradoxes is extremely important for the progress of science in many respects. Philosophically speaking, we are dealing with the apophatic pattern of the scientific study.

First and foremost, the SDRI is a set of thermodynamic paradoxes. Not more than that—but not less than that either. At the same time, the discovery of the SDRI paradoxes demanded essential further developments of powerful technical languages of compatibility conditions of singular fields as well as its implementation into multidimensional variational calculus. To the best of this author’s knowledge, still, 35 years after its appearance, these techniques have been mastered by less than 5 individuals worldwide. In fact, there is nothing paradoxical—the real pace of the progress with fundamentals is always extremely slow.

Despite the fact that SDRI of phase interfaces is a set of physical artifacts, the associated technical tools can and should be used in different applied areas of physics, mathematics, and mechanics (but, of course, not in the context of the SDRI of phase interfaces in crystalline materials). In particular, numerical modelers and computational physicists noticed in early 1990s that the SDRI, in their late stage, lead to the appearance of cracks. That observation seemed promising for developing a novel approach to formulating practically useful models of cracking.

In the terminal ballistics and many other potential applications, to which this author, has no direct relation, the mathematics of the SDRI can be immediately applied to reproduce the patterns typical for the paradox of radial cracking. However, one has clearly distinguish the mathematics of the SDRI (which is absolutely correct!) from the physics of the SDRI of phase interfaces (which is just a physical artifact!). Each publication, relating to the SDRI-based approach to radial cracking, not emphasizing clearly and explicitly this remarkable discrepancy, would indoctrinate practitioners with conceptually wrong and misleading vision. It is really unwise to erect an important technical approach using a theoretical artifact as its basis.

I think, the most productive strategy would be the following. The SDRI should preserve its status of a fundamental paradox. Then, theorists will be prompted to resolve this paradox—that is the primary practical role of any paradox. At the same time, keeping the productivity of the SDRI-based vision in mind, we have to try to modify somewhat both the physical model and the mathematical technique of the SDRI. The PMD theory is one of the possible outcomes of such an approach. The PMD does not mention explicitly or implicitly any phase-transformations whatsoever. It does not mention explicitly the SDRI whatsoever. It does not use directly any techniques associated with the SDRI theory and even with the Gibbs’³ paradigm. Yet, it uses the clear variational paradigm, typical for the classical statics. Instead of the SDRI, it uses a more traditional concept of thermodynamic instability. It allows to reproduce the radial cracking pattern.

Keeping this promising progress in mind, we might begin thinking of enriching the original simple PMD model with additional physical features. In this report, we formulate the extension of the PMD theory allowing one to include ponderomotive electrostatic or magnetostatic forces into the general scheme.

In this report, we formulate the extension of the PMD theory allowing one to include ponderomotive electromagnetic forces in the general scheme. Our approach of including the ponderomotive forces is based on earlier publications.^{5–7} One of our ultimate goals, as we foresee it now, is to suggest a novel model of electric breakdown^{8,9} based on the extended PMD approach.

There are thousands of publications devoted to analysis of ponderomotive forces including classical textbooks^{10–13} among others. The specific feature of those publications is the analysis of the problem in the framework of linear elasticity. Toupin¹⁴ was one who started the analysis in the full nonlinear framework. In our opinion, he made a strategical mistake though, relying on usage of the Lagrangian framework. Thus, he considerably narrowed the applicability of his theory since the domain, occupied by the substance, typically has a negligible size as compared with the whole space occupied by the electromagnetic field. Unfortunately, his mistake was made by many of his followers.

The approach that is presented in the work found in references 5–7 and 15 relies on the usage of the Eulerian description and it is free of the drawbacks mentioned in the Lagrangian approach of Toupin and his followers.

2. Quasi-Static Master System for Deformable Polarizable Solids

Consider a deformable polarizable substance in a thermostat maintained at fixed temperature T° . In what follows the parameter T° will be omitted from all the relationships. The free energy ψ per unit mass is given by the following formula

$$\psi = \psi(\nabla_i U_j, P^k, \kappa_M), \quad (1)$$

where P^k —the polarization vector, U_i —the displacement vector, κ_M —the damage parameters.

This substance reacts on the external load by generating elastic strain $\nabla_i U_j$ and electric polarization P^k . Under the action of these agents the integrity bonds of the substance gets broken. Since there are different bonds in solids it might be worthwhile to use different damage parameters. In the following though, we will use for brevity only 1 damage parameter κ .

We assume that the mechanical and electrostatic equilibrium in the system establishes much faster as compared with the time-scale of establishing “chemical” equilibrium. As before, by chemical equilibrium we understand the equilibrium with respect to variation in the magnitude of the damage parameter κ .

We suggest analyzing a slow evolution of this system with the help of the following master system. This system includes the system of electrostatics, consisting of the bulk equations:

$$\nabla_i D^i = 0 \quad (2)$$

and

$$z^{ijk} \nabla_j E_k = 0, \quad (3)$$

where E^i and D^i are the electrostatic field and displacement, satisfying the identity

$$D^i = E^i + 4\pi P^i. \quad (4)$$

At the internal and external boundaries these vectors should satisfy the following boundary conditions:

$$\left[E^i \right]_{-}^{+} Q_i = 0 \quad (5)$$

and

$$\left[D^i \right]_{-}^{+} N_i = 0, \quad (6)$$

where Q_i and N_i are the tangent and normal vectors to the boundary.

The bulk equations of the electrostatic and mechanical equilibrium read

$$\rho \frac{\partial \psi}{\partial P^i} = E_i \quad (7)$$

and

$$\nabla_m \aleph^{mk} = 0, \quad (8)$$

where the Aleph tensor \aleph^{mk} is defined as follows:

$$\aleph^{mk} \equiv \rho \frac{\partial \psi}{\partial \nabla_m U_j} \left(\delta_j^k - \nabla_j U^k \right) - z_{..}^{mk} \left(\frac{1}{4\pi} E_l D^l - \frac{1}{8\pi} E_l E^l \right) + \frac{1}{4\pi} D^m E^k \quad (9)$$

(see references 5–7 and 15).

By definition, at the coherent interface the displacement vector should be continuous

$$\left[U^i \right]_{-}^{+} = 0 \quad (10)$$

together with normal components of the Aleph tensor

$$\left[\aleph^{mk} \right]_{-}^{+} N_m = 0. \quad (11)$$

The same condition (Eq. 11) should be satisfied at the interface substance/vacuum (obviously, the free energy of the vacuum should be ignored).

At last, we postulate the following equation for the rate of damage:

$$\frac{\partial \kappa(z, t)}{\partial t} + V^i \nabla_i \kappa = -K \frac{\partial \psi(\nabla_i U_j, P^k, \kappa)}{\partial \kappa}, \quad (12)$$

where $V^i(z, t)$ is the velocity field of substance satisfying the identity

$$\frac{\partial U^i(z, t)}{\partial t} = V^j (\delta_j^i - \nabla_j U^i). \quad (13)$$

Here K is the rate of kinetics state function. It should be chosen based on existing experimental data. The only universal constraint on it is the positivity: $K > 0$. Also, from comparison with experimental data one has to choose the free-energy density function $\psi = \psi(\nabla_i U_j, P^k, \kappa)$. Of course, it is natural to demand that the system Equations 1–13 obeys the laws of thermodynamics. This demands imposing some constraints on the admissible functions $\psi = \psi(\nabla_i U_j, P^k, \kappa)$. These constraints are known as thermodynamic inequalities. Still, a lot of freedom remains in the choice of $\psi(\nabla_i U_j, P^k, \kappa)$. Thermodynamics is helpless in generating further constraints.

3. The PMD of Nonpolarizable Deformable Solids

For this special case, the energy density does not depend upon the polarization vector

$$\psi = \psi(\nabla_i U_j, \kappa) \quad (14)$$

the general master system reduces to the following:

$$\nabla_m \aleph^{mk} = 0, \quad (15)$$

where the Aleph tensor \aleph^{mk} reduces to the following form:

$$\aleph^{mk} \equiv \rho \frac{\partial \psi}{\partial \nabla_m U_j} (\delta_j^k - \nabla_j U^k), \quad (16)$$

which is nothing but the Cauchy stress tensor in the Eulerian variables (see reference 4 and the references therein).

By definition, at the coherent interface the displacement vector should be continuous

$$[U^i]_-^+ = 0 \quad (17)$$

together with normal components of the Aleph tensor

$$\left[\aleph^{mk} \right]_{-}^{+} N_m = 0. \quad (18)$$

The same condition (Eq. 11) should be satisfied at the interface substance vacuum (the free energy of the vacuum should be ignored).

And finally, we postulate the following equation for the rate of damage:

$$\frac{\partial \kappa(z, t)}{\partial t} + V^i \nabla_i \kappa = -K \frac{\partial \psi(\nabla_i U_j, \kappa)}{\partial \kappa}, \quad (19)$$

where $V^i(z, t)$ is the velocity field of substance satisfying the identity

$$\frac{\partial U^i(z, t)}{\partial t} = V^j (\delta_j^i - \nabla_j U^i). \quad (20)$$

Thus, in addition to the exact nonlinear master system of the PMD in the Lagrangian framework^{16–18}, we attained the exact nonlinear master system of the PMD in the Eulerian framework.

4. Quasi-Static Master System for Rigid Polarizable Solids

The above system remains meaningful even in the case of rigid (i.e., nondeformable) substances. In this case, the general master system for deformable polarizable substances reduces to the following:

$$\psi = \psi(P^k, \kappa) \quad (21)$$

$$\nabla_i D^i = 0 \quad (22)$$

$$z^{ijk} \nabla_j E_k = 0, \quad (23)$$

where E^i and D^i are the electrostatic field and displacement, satisfying the identity

$$D^i = E^i + 4\pi P^i. \quad (24)$$

At the internal and external boundaries these vectors should satisfy the following boundary conditions:

$$\left[E^i \right]_{-}^{+} Q_i = 0 \quad (25)$$

$$\left[D^i \right]_{-}^{+} N_i = 0, \quad (26)$$

where Q_i and N_i are the tangent and normal vectors to the boundary.

The bulk equations of the electrostatic and mechanical equilibrium read

$$\rho \frac{\partial \psi}{\partial P^i} = E_i . \quad (27)$$

Also, we postulate the following equation for the rate of damage:

$$\frac{\partial \kappa(z, t)}{\partial t} = -K \frac{\partial \psi(P^k, \kappa)}{\partial \kappa} \quad (28)$$

In this case, the density ρ in Eq. 27 is just an unchangeable constant.

5. The PMD for the Linear Isotropic Substances

Consider the simplest free energy density of rigid dielectrics

$$\psi(P^k, \kappa) = \frac{2\pi}{\varepsilon(\kappa) - 1} z_{jk} P^j P^k + C(\kappa) . \quad (29)$$

Then, thermodynamics imply

$$\begin{aligned} E^i(P^k, \kappa) &= \frac{4\pi}{\varepsilon(\kappa) - 1} P^i , \\ D^i(P^k, \kappa) &\equiv E^i + 4\pi P^i = \frac{4\pi\varepsilon(\kappa)}{\varepsilon(\kappa) - 1} P^i = \varepsilon(\kappa) E^i . \end{aligned} \quad (30)$$

The electrochemical master system reads

$$\frac{\partial \kappa}{\partial t} = -K \left(\frac{1}{8\pi} E^j E_j \varepsilon_\kappa(\kappa) + C_\kappa(\kappa) \right) , \quad (31)$$

and

$$\nabla_i (\varepsilon E^i) = 0 . \quad (32)$$

Let us choose the simplest model

$$\varepsilon(\kappa) = 1 + \varepsilon^\circ (1 - \alpha\kappa), \quad C(\kappa) = \frac{\chi}{2} (\kappa - \kappa^\circ)^2 . \quad (33)$$

Then, the system can be rewritten as

$$\frac{1}{K} \frac{\partial \kappa}{\partial t} = \varepsilon^\circ \alpha \frac{1}{8\pi} E^j E_j - \chi (\kappa - \kappa^\circ) , \quad (34)$$

and

$$\nabla_i \left\{ \left(1 + \varepsilon^\circ (1 - \alpha \kappa^\circ) \right) E^i \right\} = 0. \quad (35)$$

6. Spatially Uniform Equilibrium Configuration

$$\frac{\varepsilon^\circ \alpha}{4\pi} E^{*j} E_j^* = \chi (\kappa^* - \kappa^\circ) \quad (36)$$

implying

$$\kappa^* = \kappa^\circ + \frac{\varepsilon^\circ \alpha}{4\pi \chi} E^{*j} E_j^*, \quad (37)$$

and

$$\varepsilon^* = 1 + \varepsilon^\circ (1 - \alpha \kappa^\circ) - \frac{\varepsilon^{\circ 2} \alpha^2}{4\pi \chi} E^{*j} E_j^*. \quad (38)$$

For negligibly small initial damage κ° we get, respectively, the following values of the damage and electric permittivity

$$\kappa^* = \frac{\varepsilon^\circ \alpha}{4\pi \chi} E^{*j} E_j^*, \quad (39)$$

and

$$\varepsilon^* = 1 + \varepsilon^\circ - \frac{\varepsilon^{\circ 2} \alpha^2}{4\pi \chi} E^{*j} E_j^*. \quad (40)$$

7. System of Small Disturbances in Vicinity of Spatially Uniform Configuration

We obtain the system of small disturbances in vicinity of the uniform equilibrium configuration by linearizing the bulk master system (Eqs. 31 and 32). We get

$$\frac{1}{K} \frac{\partial \tilde{\kappa}}{\partial t} = \varepsilon^\circ \alpha \frac{1}{4\pi} E^{*j} \tilde{E}_j - \chi \tilde{\kappa}, \quad (41)$$

and

$$\nabla_i \left(-\alpha \tilde{\kappa} \varepsilon^\circ E^{*i} + \varepsilon^* \tilde{E}^i \right) = 0. \quad (42)$$

In 1-dimensional case the system (Eqs. 41 and 42) reads, respectively, as

$$\frac{1}{K} \frac{\partial \tilde{\kappa}}{\partial t} = \frac{\varepsilon^\circ \alpha}{4\pi} E^* \tilde{E} - \chi \tilde{\kappa}, \quad (43)$$

and

$$-\alpha \tilde{\kappa} \varepsilon^\circ E^* + \varepsilon^* \tilde{E} = A(t). \quad (44)$$

We are looking for solutions of the linear system (Eqs. 43 and 44) in the form

$$\tilde{\kappa}(x, t) = P e^{\eta t + i k x}, \quad \tilde{E}(x, t) = Q e^{\eta t + i k x}, \quad (45)$$

where k is the spatial wave-vector, η is the rate of growth of small disturbances, whereas P and Q are constants.

Substituting Eq. 45 in Eqs. 43 and 44, we get

$$\left(\frac{\eta}{K} + \chi \right) P - \frac{\varepsilon^\circ \alpha}{4\pi} E^* Q = 0, \quad (46)$$

and

$$\alpha \varepsilon^\circ E^* P - \varepsilon^* Q = 0. \quad (47)$$

The linear system (Eqs. 46 and 47) with respect to the constants P and Q has nonvanishing solutions only when its determinant vanishes. Equating the determinant to zero we arrive at the secular equation:

$$\left(\frac{\eta}{K} + \chi \right) \varepsilon^* - \frac{\varepsilon^{\circ 2} \alpha^2}{4\pi} E^{*2} = 0. \quad (48)$$

In view of Eq. 47, we arrive at the following formula for the rate η of the bulk disturbances:

$$\frac{\eta}{K} = -\chi + \frac{\varepsilon^{\circ 2} \alpha^2}{4\pi \varepsilon^*} E^{*2}. \quad (49)$$

When the rate of growth η is less than zero the disturbances decay exponentially. When η is greater than zero they grow exponentially in time. Because of this exponential growth the amplitudes of the disturbances become so big that the linearization becomes invalid. However, the linear analysis, on its own, allows to conclude that the uniform configuration becomes unstable.

The formula in Eq. 49 clearly demonstrates the competition in the influences between the chemistry of the bond's damage and ponderomotive forces. The chemistry of the bond's damage produces the stabilizing effects, whereas the ponderomotive forces try to destabilize the system by enhancing the damage. We call as critical the electric field at which the rate η crosses the zero (neutral) value. Using Eq. 50 we arrive at the following formula of the E_{crit}

$$E_{crit}^2 = \chi \frac{2\pi}{\varepsilon^{\circ 2} \alpha^2} \left(1 + \varepsilon^{\circ} (1 - \alpha \kappa^{\circ}) \right). \quad (50)$$

In the case of the small initial damage κ° the last formula reads

$$E_{crit}^2 = \chi \frac{2\pi}{\alpha^2} \frac{1 + \varepsilon^{\circ}}{\varepsilon^{\circ 2}}. \quad (51)$$

8. Conclusions

We discussed a phenomenological variational approach to the problems of electrostatics and magnetostatics. Although we explicitly focused on electrostatic heterogeneous systems, almost all of the presented results are valid for magnetostatics. Our approach is close to the Gibbs'³ minimum energy approach, as it was interpreted in Grinfeld 1994.⁴

Although the suggested approach is based on logically consistent derivation from the Gibbs'³ energy principle, its implications should not be treated as reliable physical facts. Potentially, the discrepancy of many of those implications against experiments and observations should be treated as paradoxes. We believe that it is important to remember that paradoxes always played an extremely important role in the development of fundamentals of physical sciences.

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